NRL Report 7003

CDC 3800 Computer Program to Calculate and Plot the Compressibility, Modulus of Compressibility, and Perpendicular Component of the Molecular Dipole Moment of Films Spread on Liquid Surfaces

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December 31, 1969

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ABSTRACT

A program of interest to surface chemists has been developed for use on NRL's Control Data Corporation 3800 computer. The program reads film pressure, surface potential, and molecular area data. Tabulated values are returned for the compressibility, modulus of compressibility, and perpendicular component of the molecular dipole moment, along with corresponding molecular areas. Library routines for the Calcomp Plotter are used to plot the compressibility vs area/molecule, modulus of compressibility vs area/molecule, and perpendicular component of the molecular dipole moment vs area/molecule.

PROBLEM STATUS

This is an interim report; work is continuing on the problem.

AUTHORIZATION

NRL Problem C02-10
Project RR 001-01-43-4751

Manuscript submitted October 10, 1969.

CDC 3800 COMPUTER PROGRAM TO CALCULATE AND PLOT THE COMPRESSIBILITY, MODULUS OF COMPRESSIBILITY, AND PERPENDICULAR COMPONENT OF THE MOLECULAR DIPOLE MOMENT OF FILMS SPREAD ON LIQUID SURFACES

INTRODUCTION

Much of the data collected in the study of films spread on liquid surfaces is in the form of either film pressure or surface potentials at various molecular areas. The interpretation of these data may indicate conformation and orientation of molecules in the liquid surface.

This program, titled "Films," was developed to avoid the tedious slope calculations necessary for obtaining compressibility curves from film pressure data. Because surface potential, ΔV, data are often collected along with film pressure data, the program uses ΔV data to calculate molecular dipole moments perpendicular to the liquid surface.

GENERAL PROGRAM INFORMATION

Input is grouped either as set 1 data or set 2 data, depending on whether it is film pressure vs area/molecule (set 1) or surface potential vs area/molecule (set 2). For set 1 data, the program returns tabulations and plots of the compressibility and modulus of compressibility vs area/molecule. For set 2 data, the program returns perpendicular dipole vs area/molecule.

The program may be run with either or both sets present in the data deck. All set 1 data must be kept together, and all set 2 data must be kept together. Set 1 data need not precede set 2 data in the data deck. Input may be presented in either increasing or decreasing order by area, but successive data points must be presented successively in the data deck.

The program accepts up to and including 50 points for each film pressure run and 50 points for each surface potential run. The program accepts up to and including 99 runs for each set 1 and set 2.

Output quantities are calculated as follows:

$$\text{Compressibility}_{(i)} \text{ in cm/dyne} = \frac{1}{A_{(i)}} \cdot \frac{A_{(i-1)} - A_{(i)}}{F_{(i)} - F_{(i-1)}},$$

where (i) refers to the ith data point, F is the film pressure in dynes/cm, and A is the molecular area in square angstroms/molecule.

$$\text{Modulus}_{(i)} \text{ of compressibility in dynes/cm} = \frac{1}{\text{compressibility}_{(i)}}$$

and

$$\text{Perpendicular dipole}_{(i)} \text{ in Debye units} = \frac{\Delta V_{(i)} A_{(i)}}{4\pi} \times 3 \times 10^{-4},$$

where ΔV is surface potential in millivolts.

INPUT LIMITS

Area/molecule: 0.00 to 999.99 square angstroms/molecule

Film pressure: 0.00 to 99.99 dynes/cm

Surface potential: 0.00 to 999.99 millivolts

OUTPUT LIMITS

Compressibility: no limits on magnitude but three significant digits

Modulus of compressibility: same as for compressibility

Perpendicular dipole: 0.00 to 99.99 Debye units

DEFINITIONS OF TERMS IN PROGRAM

ITSETS — the total number of data sets in the data deck. ITSETS will equal 1 if only one type of data (either set 1 or set 2) is present. ITSETS will equal 2 if both sets 1 and 2 are present in the data deck.

ITSET — designation of data type: ITSET = 1 indicates film pressure-vs-area data and ITSET = 2 indicates surface potential-vs-area data

ITRUNS — total number of experimental trials for either set 1 or set 2 data. For example, if one film-pressure-vs-area curve was made of five different compounds, ITRUNS for set 1 would equal 5. If five film pressure-vs-area curves were made of one compound, ITRUNS for set 1 would equal 5. If three film pressure-vs-area curves were made of one compound and one film pressure-vs-area curve was made of two additional compounds, ITRUNS for set 1 would equal 5.

$$0 \leq \text{ITRUNS} \leq 99$$

IRUN — ordinal number of an experimental trial in either set 1 or set 2.

$$0 \leq \text{IRUN} \leq 99$$

NUM — number of data points in some particular IRUN.

$$0 \leq \text{NUM} \leq 50$$

Information about the Calcomp Plotter subroutines used in this program can be found in the following notes and memoranda:

1. Memorandum 7810-5:ABB:rmd:pj, September 18, 1967, Plotter Subroutine Package.
2. Memorandum 4500-31:DEG:rmd, August 24, 1967, 3800 Utility Program.

3. Memorandum 7810-33:GHR:rmd, November 22, 1967, Plotter Subroutine Package.

4. Memorandum 7810-121:GR:vjs, August 14, 1968, Changes in Plotter Subroutine Package.

5. NRL Computer Note 6, October 17, 1968, Plot Time Message for the Calcomp Plotter.

6. NRL Computer Note 10, December 17, 1968, Initialization for the 3800 Calcomp Plotter Package.

7. NRL Computer Note 25, June 12, 1969, New SCALE Subroutine to go on the 3800 System Library.

PROGRAM

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      PROGRAM FILMS
      DIMENSION AREA (50),PRESS(50),COMP(50),CMOD(50),DELV(50),PERMU(50)
     1,DELA(50),DELP(50),ARRAY(254)
      CALL PLOTS (ARRAY,254,7)
       ICOUNT=0
      READ 100,ITSETS
       READ 101,ISET,ITRUNS
8     GO TO (1,2) ISET
1      DO 4 I=1,ITRUNS
      READ 102,IRUN,NUM,N,A,M,E
      NNUM=NUM-1
      DO 5 II=1,NUM
      AREA(II)=0.
      PRESS(II)=0.
5      CONTINUE
      DO 6 II=1,NUM
      READ 103, AREA(II),PRESS(II)
6      CONTINUE
      DO 7 II=2,NUM
      DELA(II)=AREA(II-1)-AREA(II)
      DELP(II)=PRESS(II)-PRESS(II-1)
      COMP(II)=(1./AREA(II))*(DELA(II)/DELP(II))
      CMOD(II)=1./COMP(II)
7      CONTINUE
      PRINT 200,ISET,IRUN,N,A,M,E
      DO 9 J=1,NUM
      PRINT 201,PRESS(J),AREA(J)
9      CONTINUE
      PRINT 202
      DO 10 J=2,NUM
      PRINT 203,COMP(J),CMOD(J),AREA(J)
10      CONTINUE
      CALL SCALE(COMP(2),NNUM,8.,CMIN,DC,1,CTK)
      CALL AXIS(0.,0.,25HCOMPRESSIBILITY (CM/DYNE),25,8.,90.,CTK,CMIN,
     1DC,5HE10.3)
      CALL SCALE(AREA(2),NNUM,10.,AMIN,DA,1,ATK)
      CALL AXIS(0.,0.,28HAREA/MOLECULE (SQ.ANGSTROMS),-28,10.,0.,ATK,
     1AMIN,DA,4HF6.2)
       CALL PLOT (0.,0.,2)
      CALL LINE (AREA(2),COMP(2),NNUM,1,2,0,1,1)
      CALL PLOT(1.,10.,3)
      CALL PLOT(1.,10.,2)
      CALL SYMBOL (1.,10.,0.21,21HCOMPRESSIBILITY CURVE,0.,21)
      CALL PLOT(10.,0.,-3)
      CALL SCALE(CMOD(2),NNUM,8.,CMMIN,DCM,1,CMTK)
      CALL AXIS(0.,0.,17HMODULUS (DYNE/CM),17,8.,90.,CMTK,CMMIN,DCM,
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     15HE10,3)
      CALL AXIS (0,,0,,28HAREA/MOLECULE (SQ,ANGSTROMS),-28,10,,0,,ATK,
     1AMIN,DA,4HF6,2)
      CALL PLOT(0,,0,,2)
      CALL LINE (AREA(2),CMOD(2),NNUM,1,1,0,1,1)
      CALL PLOT(1,,10,,3)
      CALL PLOT(1,,10,,2)
      CALL SYMBOL (1,,10,,0,21,26HMODULUS OF COMPRESSIBILITY,0,,26)
      CALL PLOT (13,,0,,-3)
4      CONTINUE
      ICOUNT=ICOUNT+1
20      IF (ITSETS .EQ. 1) GO TO 500
      IF (ICOUNT .EQ.2) GO TO 500
       READ 101,ISET,ITRUNS
      GO TO 8
2      DO 15 I=1,ITRUNS
      READ 102,IRUN,NUM,N,A,M,E
      DO 16 II=1,NUM
      AREA (II)=0,
      DELV(II)=0,
16      CONTINUE
      DO 13 II=1,NUM
      READ 103, AREA(II),DELV(II)
      PERMU(II)=(DELV(II)*AREA(II)/(4,*3,14159))*3,*(10,**(-4))
13      CONTINUE
      PRINT 204,ISET,IRUN,N,A,M,E
      DO 11 II=1,NUM
      PRINT 201,DELV(II),AREA(II)
11      CONTINUE
      PRINT 205
      DO 12 II=1,NUM
      PRINT 206,PERMU(II),AREA(II)
12      CONTINUE
      CALL SCALE (PERMU, NUM,8,,PMIN,DP,1,PTK)
      CALL AXIS (0,,0,,15HDIPOLE (DEBYES),15,8,,90,,PTK,PMIN,DP,4HF4,2)
      CALL SCALE (AREA,NUM,10,,AMIN,DA,1,ATK)
      CALL AXIS (0,,0,,28HAREA/MOLECULE (SQ,ANGSTROMS),-28,10,,0,,ATK,
     1AMIN,DA,4HF6,2)
      CALL PLOT (0,,0,,2)
      CALL LINE (AREA,PERMU,NUM,1,0,0,1,1)
      CALL PLOT (1,,10,,3)
      CALL PLOT (1,,10,,2)
       CALL SYMBOL (1,,10,,0,21,20HPERPENDICULAR DIPOLE,0,,20)
       CALL PLOT (13,,0,,-3)
15      CONTINUE
      ICOUNT=ICOUNT+1
       GO TO 20
100    FORMAT (I1)
101    FORMAT (I1,5X,I2)
102      FORMAT (I2,5X,I2,5X,A8,A8,A8,A8)
103    FORMAT (F6,2,5X,F6,2)
200    FORMAT(//,27X,20HORIGINAL DATA:  SET=,I1,2X,4HRUN=,I2,2X,4A8/
     138X,23HFILM PRESSURE(DYNES/CM),5X,28HAREA/MOLECULE(SQ, ANGSTROMS)/
     2)
201      FORMAT (47X,F6,2,25X,F6,2)
202    FORMAT (//,58X,15HCALCULATED DATA/17X, 24HCOMPRESSIBILITY(CM/DYNE
     1),5X,35HMODULUS OF COMPRESSIBILITY(DYNE/CM),5X,28HAREA/MOLECULE(SQ
     2, ANGSTROMS)/)
203      FORMAT (24X,E10,3,25X,E10,3,30X,F6,2)
204    FORMAT(///,28X,20HORIGINAL DATA:  SET=,I1,2X,4HRUN=,I2,2X,4A8/
     137X,25HDELTA VOLTAGE(MILLIVOLTS),5X,28HAREA/MOLECULE(SQ, ANGSTROMS
     2)/)
205    FORMAT (//,58X,15HCALCULATED DATA/35X, 28HPERPENDICULAR DIPOLE(DE
     1BYES),5X,28HAREA/MOLECULE(SQ, ANGSTROMS)/)
206    FORMAT (45X,F4,2,38X,F6,2)
500     CALL STOPPLOT
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Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author)	2a. REPORT SECURITY CLASSIFICATION
Naval Research Laboratory Washington, D.C. 20390	Unclassified
	2b. GROUP

3. REPORT TITLE

CDC 3800 COMPUTER PROGRAM TO CALCULATE AND PLOT THE COMPRESSIBILITY, MODULUS OF COMPRESSIBILITY, AND PERPENDICULAR COMPONENT OF THE MOLECULAR DIPOLE MOMENT OF FILMS SPREAD ON LIQUID SURFACES

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

Interim report; work is continuing on the problem.

5. AUTHOR(S) (First name, middle initial, last name)

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6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
December 31, 1969	7	

8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S)
NRL Problem C02-10 b. PROJECT NO. RR 001-01-43-4751 c. d.	NRL Report 7003 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)

10. DISTRIBUTION STATEMENT

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11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
	Department of the Navy (Office of Naval Research), Washington, D.C. 20360

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DD FORM 1 NOV 65 1473 (PAGE 1)

S/N 0101-807-6801

Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Computers						
Surface properties						
Compressibility						
Modulus of compressibility						
Dipole moment						
Monomolecular films						